Final Technical Report:
NAG3-2493   The Dynamics of Miscible Interfaces: Simulations
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The goal of this experimental/computational investigation (joint with Prof. Maxworthy at USC) has been to study the dynamics of miscible interfaces, both from a scientific and a practical point of view, and to prepare a related experiment to be flown on the International Space Station. The interest is in unraveling a number of difficult problems that have arisen in the study of miscible interfaces. When two fluids, with different densities, are in relative motion and interdiffuse, the resulting equations of motion contain effects that are not present in more conventional systems. Even if the two fluids are incompressible, the usual mass-averaged velocity is not divergence free in the mixing region. However, previous computational simulations of such flows routinely assume this effect to be small (without providing a quantitative estimate for its size), and they employ a non-divergent velocity field. Obviously, it is important to establish the range of validity of this approach. In addition, as discussed primarily by Joseph and coauthors, other so-called Korteweg stresses could be important in regions of large concentration gradients. Not only the magnitude of the coefficients in these stresses, but also their sign, are presently unknown, although some rough estimates exist in the literature. Hence there is a fundamental motivation to clarify the role of these stresses. This research also has a practical motivation, since the improved understanding of the dynamics of multiphase porous media flows is a prerequisite for progress in the fields of enhanced oil recovery, hydrology, filtration etc. In order to address these effects, we have focused experimental and computational investigations on miscible displacements in cylindrical capillary tubes, as well as in Hele-Shaw cells. Part of the experimental component was conducted with our collaborator Dr. Petitjeans at ESPCI, Paris. Regarding the flow in a capillary tube, the question was addressed as to whether Korteweg stresses and/or divergence effects can potentially account for discrepancies observed between conventional Stokes flow simulations and experiments for miscible flows in capillary tubes. An estimate of the vorticity and streamfunction fields induced by the Kortewegs stresses was derived, which shows these stresses to result in the formation of a vortex ring structure near the tip of the concentration front. Through this mechanism the propagation velocity of the concentration front is reduced, in agreement with the experimental observations. Divergence effects, on the other hand, were seen to be very small, and they have a negligible influence on the tip velocity. As a result, it can be concluded that they are not responsible for the discrepancies between experiments and conventional Stokes simulations. A further part of our investigation focussed on the development of high-accuracy three-dimensional spectral element simulation techniques for miscible flows in capillary tubes, including the effects of variable density and viscosity. Towards this end, the conservation equations are treated in cylindrical coordinates. The spatial discretization is based on a mixed spectral element/Fourier spectral scheme, with careful treatment of the singularity at the axis. For the temporal discretization, an efficient semi-implicit method is applied to the variable viscosity momentum equation. This approach results in a constant coefficient Helmholtz equation, which is solved by a fast diagonalization method based on a Schur complement decomposition. Numerical validation data are presented, and simulations are

conducted for the three-dimensionally evolving instability resulting from an unstable density stratification in a vertical tube. Some preliminary comparisons with corresponding experiments are undertaken. In combination with the experimental component of the investigation, the preparation of the planned Space Station investigation MIDAS was advanced to the stages of the successful Science Requirement Review (May 2000), as well as the equally successful Requirements Definition Review (April 2002). As a result, the present project has been extended, and it currently continues at UCSB and USC with support from NASA. Publications that have evolved from the grant: The Dynamics of Miscible Interfaces and the Effects of Korteweg Stresses, with C.-Y. Chen and L.-L. Wang, Trans. Aero. Astro. Soc. R. O. C. 33, 7 (2001). Miscible Droplets in a Porous Medium and the Effects of Korteweg Stresses, with C.-Y. Chen and L.-L. Wang, Phys. Fluids 13, 2447 (2001). Density-Driven Unstable Flows of Miscible Fluids in a Hele-Shaw Cell, with J. Fernandez, P. Kurowski, and P. Petitjeans, J. Fluid Mech. 451, 239 (2002). Density-Driven Instabilities of Miscible Fluids in a Hele-Shaw Cell: Linear Stability Analysis of the Three-Dimensional Stokes Equations, with F. Graf and C. Haertel, J. Fluid Mech. 451, 261 (2002). Miscible Displacements in Capillary Tubes: Influence of Korteweg Stresses and Divergence Effects, with C.-Y. Chen, Phys. Fluids, July (2002). Three-dimensional spectral element simulations of variable density and viscosity, miscible displacements in a capillary tube, with D. Wilhelm, submitted to Comp. and Fluids (2002). Chemical Fronts in Hele-Shaw Cells: Linear Stability Analysis Based on the Three-dimensional Stokes Equations, with R. Demuth, submitted to Phys. Fluids (2002). The Dynamics of Miscible Interfaces and the Effects of Korteweg Stresses, with C.-Y. Chen, Proceedings of the Seventh National Computational Fluid Dynamics Conference, Kenting, Taiwan, August 2000. The Dynamics of a Miscible Interface in a Capillary Tube, with T. Maxworthy, J. Kuang, P. Petitjeans, and C.-Y. Chen, Proceedings of the Second Pan-Pacific Basin Workshop on Microgravity Sciences, Pasadena, CA, May 2001. Three-Dimensional Stability Analysis and Nonlinear Simulations of Unstably Stratified Miscible Fluids in a Hele-Shaw Cell, with F. Graf and C. Haertel, Proceedings of the Microgravity Transport Processes in Fluid, Thermal, Materials, and Biological Sciences Conference II, Banff, Canada, September 2001. The Dynamics of Miscible Fluids: A Space Flight Experiment (MIDAS), with T. Maxworthy, R. Balasubramaniam, N. Rashidnia, and R. Lauver, AIAA-Paper 2001-5061, International Space Station Utilization Conference, Kennedy Space Center, FL, October 2001. Miscible Hele-Shaw Flows: Three-Dimensional Linear Stability Results, with F. Graf and C. Haertel, AIAA-Paper 2002-0888, 40th AIAA Aerospace Sciences Meeting, Reno, NV, January 2002.